Measured a biotite compostion? Estimate *P–T* with deep learning!

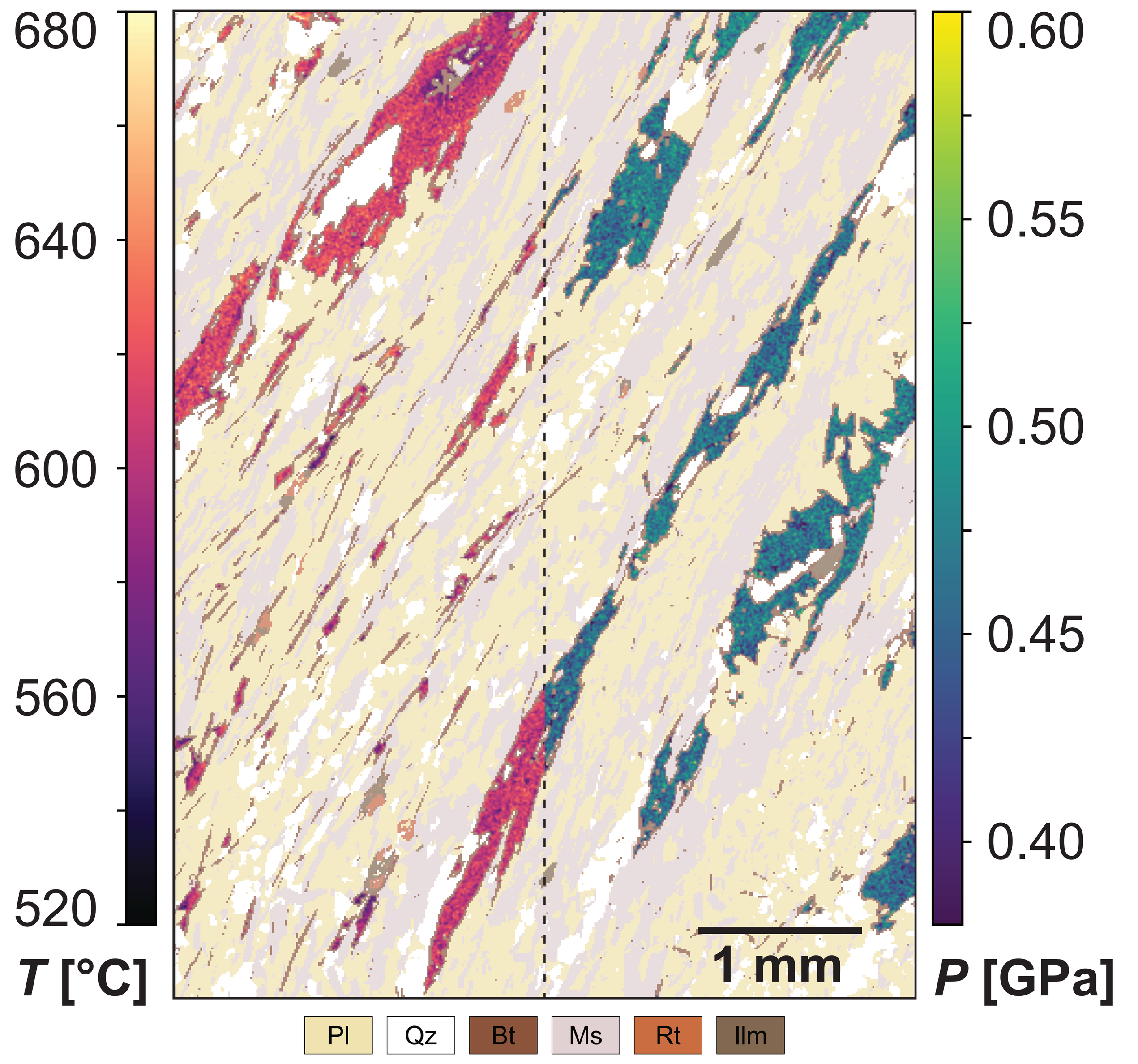


Figure 1.1 P–T predicted based on a compositional map of biotite in the metapelitic Croveo Schist from the Central Alps [1].

1. INTRODUCTION & METHODS

Challenge: *How to callibrate a metamorphic thermobarometer?*

Metamorphic thermobarometry

= Pressure (*P*)–Temperature(*T*) estimation of:
- Equilibration of a rock
- Mineral recrystallisation

Addresses fundamental petrological questions:
- Understanding geochemical processes
- Reconstructing geodynamic evolution

How to callibrate a thermobarometric funtion?

1. Fit the parameters of a reaction

Typically experimental data
- Net-transfer or exchange reactions [2,3]
- Trace element incorporation [4]

(+) Exact *P–T* (-) High *T*
(-) Simplified system

2. Statistical relation in large datasets

Natural or experimental data
- Ti-in-Bt thermometer [5,6]
- Magmatic thermometer [7,8]

(+) Natural complexity (-) Independent *P–T* needed

Use a database of natural metamorphic biotite:

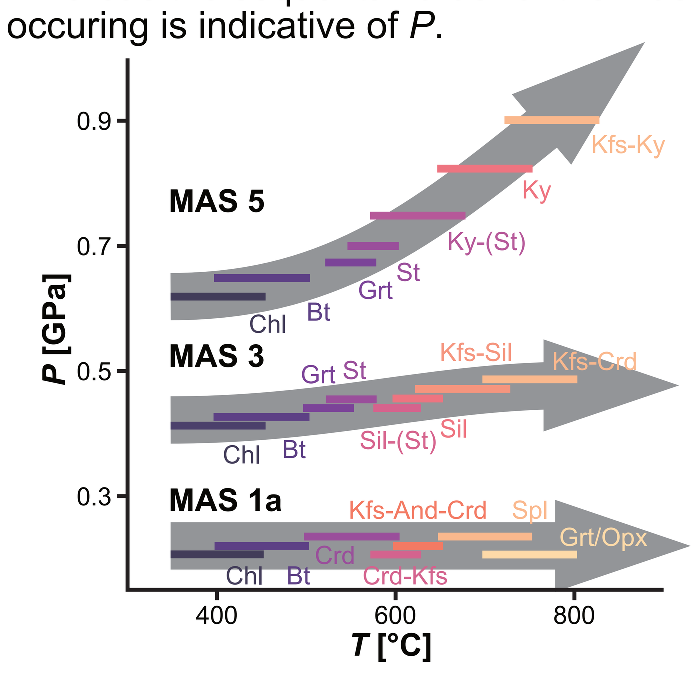
Pattison & Forshaw (in prep.)
- 2148 natural biotite analyses
- 126 metamorphic sequences

Use the systematic order of mineral occurence in metamorphic sequences to obtain *P–T* estimates[9,10]:
- *P*: Mineral assemblage sequence (MAS)
- *T*: Index mineral zone

Statistical model:
- Neural Network (syn. deep learning)

Learn more about the machine-learning algorithm in the box below.

Figure 1.2. Example of three metamorphic sequences. Index minerals define zones in *T*. Whereas the sequential order of the index minerals occuring is indicative of *P*.



2. TESTING THE THERMOBAROMETER

Challenge: *How to determine independent reference P–T estimates to test predictions against?*

Sample TG8C-03

Granulite-facies metapelite from Higher Himalayan Crystalline Sequence (Sikkim, India) [11,12].

Reference peak *P–T* from iterative thermodynamic modelling (Bingo-Antidote) [13]:

***T* = 790 °C** and ***P* = 0.64 GPa**

Two biotite compositions from different cogenetic assemblages present in the samples.

Propagate compositional variance to *P–T* estimates:

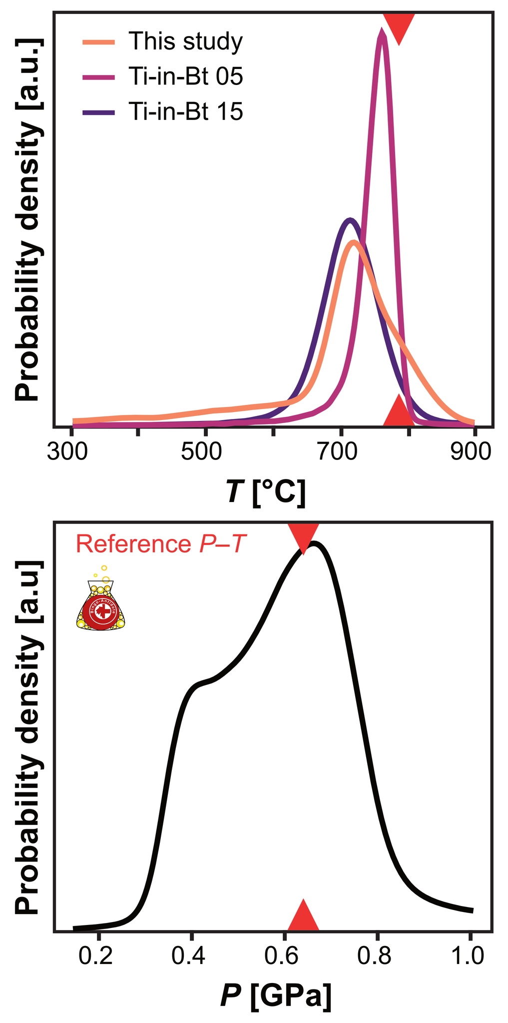


Figure 2.1. Distribution of *P–T* estimates for TG8C-03. Red triangles mark reference metamorphic conditions determined by iterative thermodynamic modelling [13]. For *T* estimates by the two Ti-in-Bt [5,6] thermometers are shown as comparison.

Samples with multiple lines of evidence

TG8C-03 + 8 samples with reference *P–T* from:
- Phase equilibrium modelling
- Iterative thermodynamic modelling
- Empirical thermobarometer
- Non-traditional thermobarometry (QuiG, Zr-in-Rt)

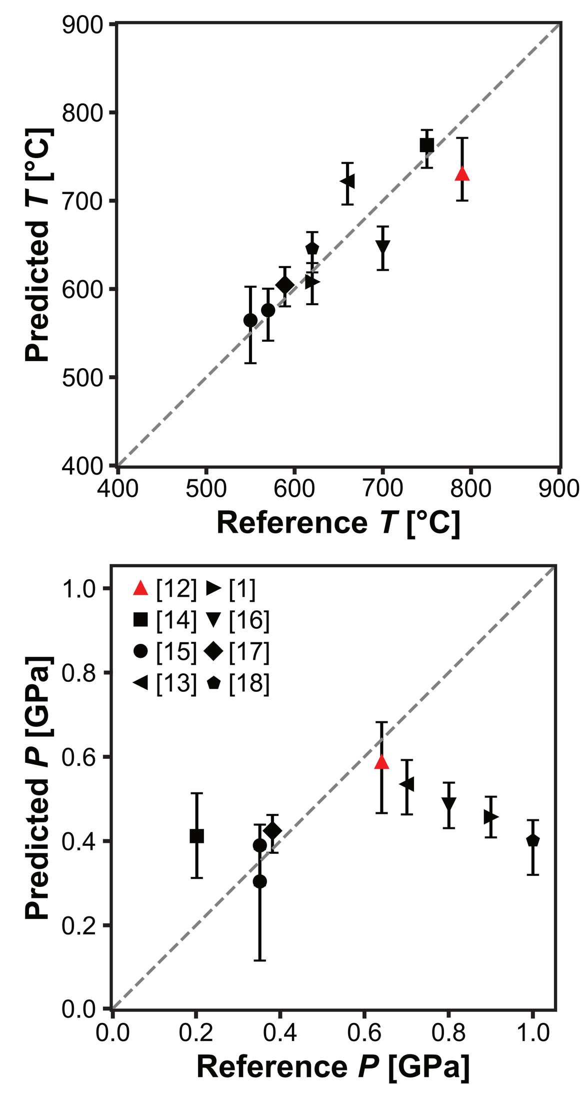


Figure 2.2. Comparison of the *P–T* predicted by the biotite thermobarometer and the conditions reported by the original authors for the a test set of nine samples.

Metamorphic sequences:

Individual estimates for *P–T* are unprecise.

The sequential relation of samples adds the additional constraint, that *T* must increase upgrade.

Accuracy check of *P–T* estimates
- Over wide *P–T* range
- Assert systematic errors

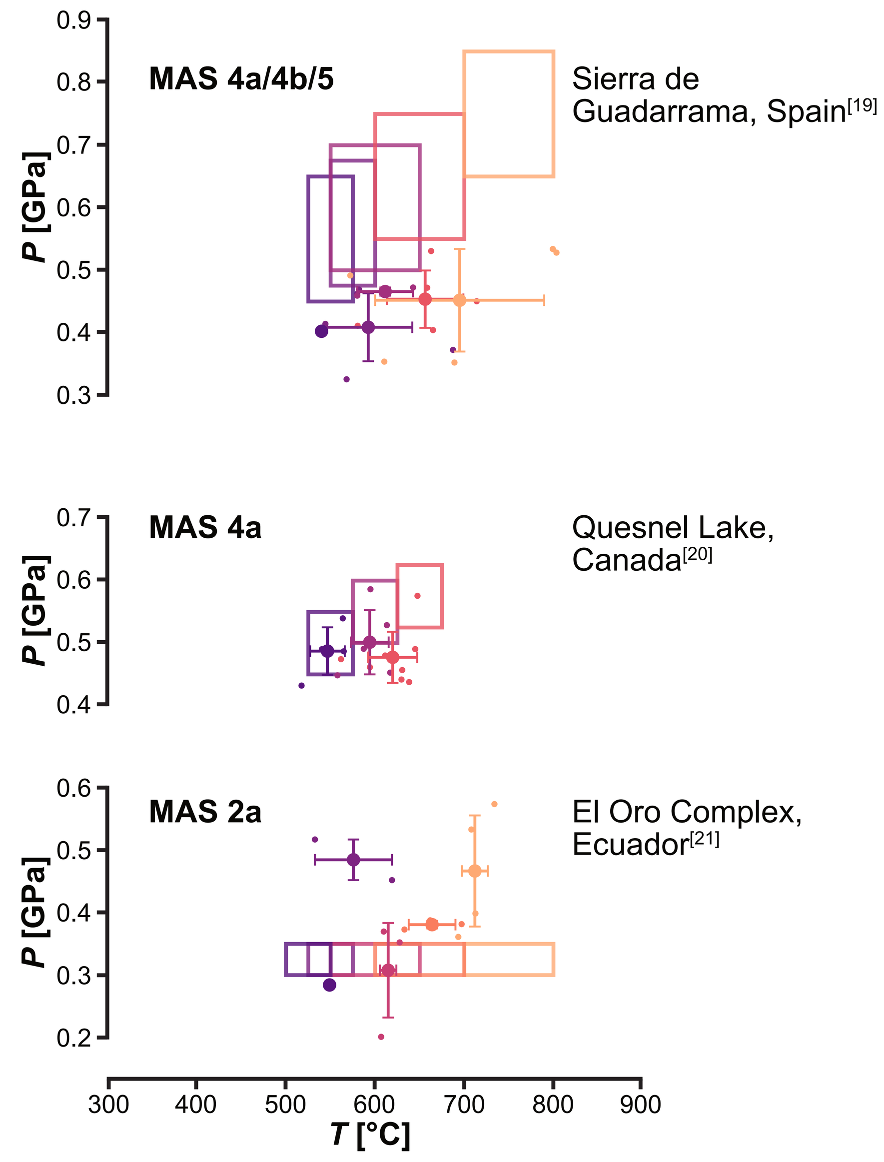


Figure 2.3. Predicted *P–T* for biotites from three metamorphic sequences tested. Boxes mark the reference *P–T* of a index mineral zone in a MAS after Pattison & Forshaw (in prep.). If multiple biotites were measured in one zone the mean *P–T* and standard deviation are shown ontop of the individual predictions. For all sequences the predicted *T* increases upgrade as expected and overlaps with the reference. *P* is overestimated in the low *P* sequence (MAS 2a) and underestimated in the high *P* sequence (MAS 4a/4b/5). These discrepancies may result form inherent complexity and polymetamorphism in the sequences used to callibrate and test the thermobarometer.

3. CONCLUSION

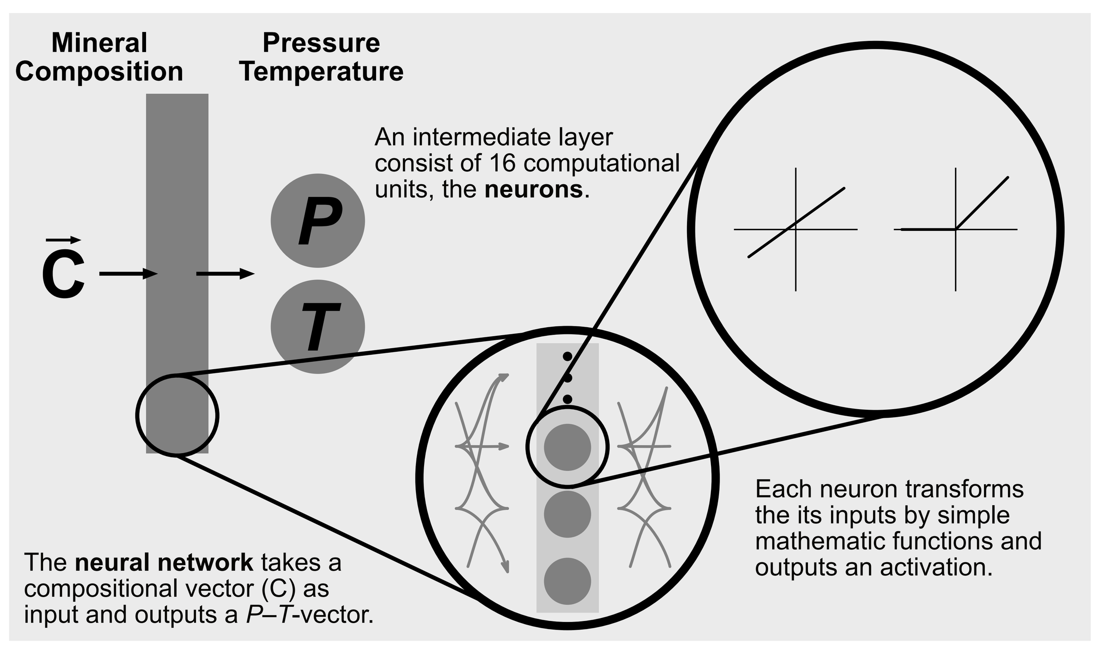
Metamorphic sequences can be used to approximate a thermobarometric function. → Developed a coupled biotite thermobarometer using deep learning.

Thermobarometer can be tested using samples with differnet independently determined *P–T* estimates. →
- Precise and accurate thermometer:

  Δ*T* = ± 29 °C
- Barometer can provide rough estimate:

  Δ*P* ≈ ± 0.2 GPa
- Systematic underestimation of *P* > 0.65 GPa

Deep Learning



Each neuron is a **linear transformation**, followed by a non-linear **activation function**.

Train by fitting parameters of linear part:
- Weights (slope)
- Biases (intercept)

Complex functions emerge by
1. Neurons working in parallel
2. Concatenating layers of neurons

For an optimal performance **hyperparameters** must be tuned by systematic testing on a validation dataset.

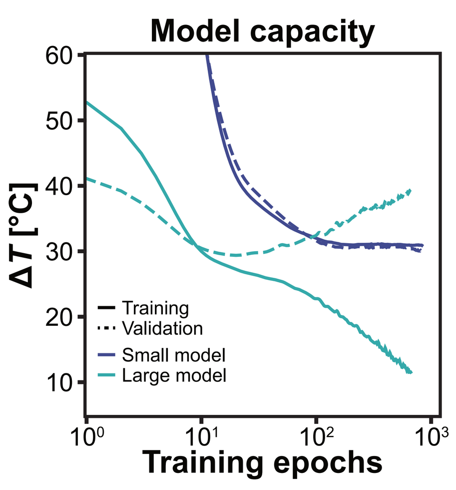


Figure 4.1. Effect of different model capacities on the perfomance. A larger model, with more trainable parameters, can approximate relations in the training dataset better. By overfitting to the training data its performance on a validation set decreases with training. The learned function is not a generally valid thermobarometer.

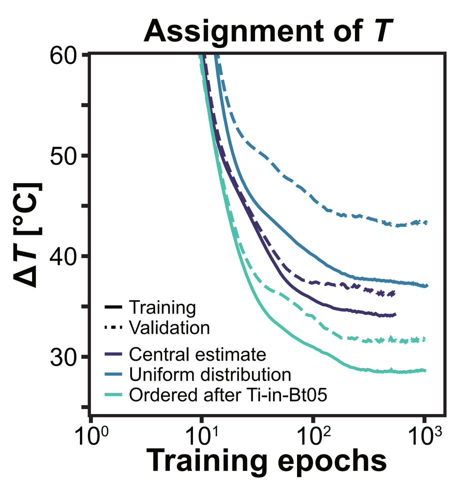


Figure 4.2. Different methods to assign *P–T* based on a zone/MAS pair the natural data were tested: (1) a central estimate for *P* and *T*, (2) random sampling *P* and *T* from a uniform distribution, (3) random sampling *T* from a distribtuion ordered after Ti-in-Bt [5].

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Thermobarometry using machine-learning
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